Developing a Solid State Electrolyte for Advanced Lithium Batteries

Completed Technology Project (2017 - 2021)

Project Introduction

Lithium ion batteries currently use an organic electrolyte that is flammable and raises major safety concerns. One method to enable safer and more energy dense batteries is to replace this electrolyte with a solid state material. Before solid state electrolytes (SSEs) can be realized, they much have low resistance and be nonreactive with the anode material: lithium. Traditional SSE materials have reacted with lithium forming a passivation layer called the solid electrolyte interface (SEI) which leads a decrease in efficiency over times. Another key concern is the formation of dendrites (needle-like structures) in the grain boundaries of the SSE formed during repeated cycling of the battery which can lead to early cell failure. The objective of this proposal is to combine experimental and computational methods to investigate a family of crystalline sulfides, Li-argyrodite Li5PS5X where X= Cl, Br, or I to develop a SSE for a lithium battery. Density functional theory calculations will allow for estimated calculations of Li diffusion coefficients to determine conductivity, and will also be used to calculate of binding energies of side reaction products to predict SEI characteristics between the SSE and lithium anode. These computer models will allow for rapid screening of different materials, structures, and geometries to determine what materials will have the largest lithium ion conductivity and what materials should be used at the SSE/lithium interface. All computational screening is verified and guided by experimental data collected through electrochemical characterization and cyclic voltammetry experiments. This proposal seeks to understand structure/property relationships of SSE materials on a fundamental level allowing for more efficient design of safer batteries. Batteries are used in almost every type of space technology from satellites and telescopes to the international space station and rovers. Weight, safety, and reliability are of paramount concern in these applications to reduce the cost of launching equipment into space, and to prevent any types of fires or failures. A solid state battery provides firstly numerous safety advantages over traditional lithium ion technologies because it does not contain a flammable liquid electrolyte. A SSE would also allow for high energy density by volume, and if the battery contains lithium metal at the anode the energy density would increase meaning lighter batteries would be required to support equipment.

Anticipated Benefits

Batteries are used in almost every type of space technology from satellites and telescopes to the international space station and rovers. Weight, safety, and reliability are of paramount concern in these applications to reduce the cost of launching equipment into space, and to prevent any types of fires or failures. A solid state battery provides firstly numerous safety advantages over traditional lithium ion technologies because it does not contain a flammable liquid electrolyte. A SSE would also allow for high energy density by volume, and if the battery contains lithium metal at the anode the energy density would increase meaning lighter batteries would be required to support

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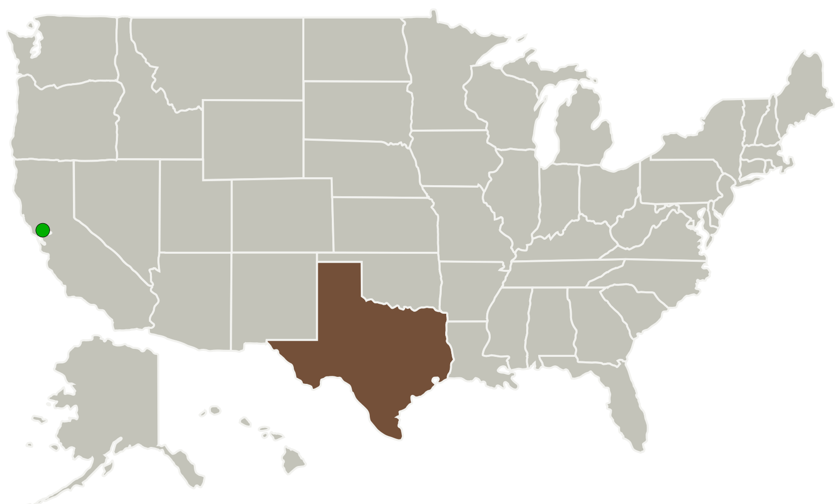
equipment.

Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
University of Houston	Lead Organization	Academia Asian American Native American Pacific Islander (AANAPISI), Hispanic Serving Institutions (HSI)	Houston, Texas
Ames Research Center(ARC)	Supporting Organization	NASA Center	Moffett Field, California

Primary U.S. Work Locations
Texas

Project Website:

https://www.nasa.gov/strg#.VQb6T0jJzyE

Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Lead Organization:

University of Houston

Responsible Program:

Space Technology Research Grants

Project Management

Program Director:

Claudia M Meyer

Program Manager:

Hung D Nguyen

Principal Investigator:

Lars Grabow

Co-Investigator:

Karun Kumar Rao

Technology Maturity (TRL)

Start: **2**
Current: **2**
Estimated End: **3**

1	2	3	4	5	6	7	8	9
Applied Research			Development			Demo & Test		

Technology Areas

Primary:

- TX03 Aerospace Power and Energy Storage
  - └ TX03.2 Energy Storage
    - └ TX03.2.1 Electrochemical: Batteries

Target Destinations

Earth, The Moon, Mars